Static Properties of Trapped Bose Gases at Finite Temperature: Thomas-Fermi Limit

M. Benarous and H. Chachou-Samet

Laboratory for Theoretical Physics and Material Physics

Faculty of Sciences and Engineering Sciences

Hassiba Benbouali University of Chlef

B.P. 151, 02000 Chlef, Algeria.

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Abstract

We rely on a variational approach to derive a set of equations governing a trapped self-interacting Bose gas at finite temperature. In this work, we analyze the static situation both at zero and finite temperature in the Thomas-Fermi limit. We derive simple analytic expressions for the condensate properties at finite temperature. The noncondensate and anomalous density profiles are also analyzed in terms of the condensate fraction. The results are quite encouraging owing to the simplicity of the formalism.

1 Introduction

In a remarkable series of experiments on Rubidium and Sodium vapors[1, 2], the Bose-Einstein condensation was first observed. Although having been predicted theoretically a long time ago for noninteracting boson systems[3], the experimental challenge was to demonstrate that a real gas can indeed be "bose condensed". Since then, a great effort was devoted by researchers all around the world in order to understand and predict the condensate properties. The main tools, beside the Monte-Carlo calculations[4], were the Bogoliubov[5], the Popov[6], the Beliaev[7, 8] and the Hartree-Fock-Bogoliubov[9, 10, 11] approximations. These approximations all adopt some simplifying assumptions about the various quantities involved in the problem, such as the order parameter Φ, or the condensate density $n_c \equiv |\Phi|^2$, the non-condensed density or thermal cloud $\tilde{n}$ and the anomalous density $\tilde{m}$. A major well-known drawback of these methods is that they cannot be easily extended to situations where their main assumptions fail. In a previous paper[12], we rely on a different approach, based on the time-dependent variational principle of Balian and Vénéroni[13] , which allows one to overcome some of those restrictions. We obtained a set of three coupled dynamical equations, which we called "Time-Dependent Hartree-Fock-Bogoliubov" (TDHFB) equations, governing the evolution of Φ, $\tilde{n}$ and $\tilde{m}$. They were shown to generalize in a consistent way the Gross-Pitaevskii equation[14].

The present paper is devoted to analyze the implications of our TDHFB equations. Since it is important to apprehend first what happens in the static situation before going further into the analysis of the excitation spectrum or to the full dynamical case, we will focus on the static solution both at zero and finite temperature in the Thomas-Fermi (TF) limit. The interest is evident, since there remain many unanswered questions such as the general dependence of the density profiles on the temperature and on the interaction strength and the effect of the interactions on the critical temperature. More particularly, recent experiments are raising challenging questions about the precise determination of the thermal cloud and its backeffects on the condensate[15]. Indeed, due to the difficulties inherent to these experiments, there is no clear image on the way the condensed and non condensed phases mix up. Hence, in these preliminary calculations, we intend to provide some simple answers. We do not pretend of course to reproduce exactly the experimental data or the full Monte-Carlo calculations, but we would like to show that the simplifications that we are actually using (Mean field + Thomas-Fermi) are controlable and retain also the most important qualitative features without destroying the underlying physics. This provides a simple enough tool which can be considered as a starting point

for a more elaborate treatment.

The paper is organized as follows. In section 2, we recall the main steps that have been used in [12] to derive the TDHFB equations. Then, we present the static solutions and discuss their properties at zero temperature. At finite temperature, the equations are much more involved and require a careful analysis. In the TF limit, we present a simple method which allows for a self-consistent determination of the various density profiles as well as some other static properties of the condensate such as the chemical potential and the condensate radius. Indeed, the TF approximation obviously provides simple enough analytical expressions since it neglects the kinetic terms thus yielding algebraic equations instead of partial differential equations. This is the main advantage of our method which yields the most important qualitative features without having to handle highly non-linear differential equations.

In section 3, we present the results of our calculations. We plot first the condensate radius and the central density as functions of the condensate fraction and note in particular the compression effect of the condensate due to the thermal cloud. Moreover, we discuss the TF profile obtained for the condensate density even at low condensate fraction. The noncondensate density profile is also plotted for a wide range of condensate fraction and shows a good qualitative agreement with recent experiments. Finally, the anomalous density, although not yet measured experimentally, is shown to behave in a quite intuitive way.

Some concluding remarks are given at the end of the paper.

2 The TDHFB Equations and Their Static Solutions

The general TDHFB equations were derived in ref.[12] for a grand canonical Hamiltonian of trapped bosons with quartic self-interactions (with coupling constant g and mass m):

$$H = \int_{\mathbf{r}} a^+(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(\mathbf{r}) - \mu \right] a(\mathbf{r}) + \frac{g}{2} \int_{\mathbf{r}} a^+(\mathbf{r})a^+(\mathbf{r})a(\mathbf{r})a(\mathbf{r}). \qquad (2.1)$$

The quantity $V_{\text{ext}}(\mathbf{r})$ is the trapping potential and μ is the chemical potential. These equations read:

$$
\begin{aligned}
i\hbar\dot{\Phi} &= \left(-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}} - \mu + gn_c + 2g\tilde{n} \right)\Phi + g\tilde{m}\Phi^*, \\
i\hbar\dot{\tilde{n}} &= g\left(\tilde{m}^*\Phi^2 - \tilde{m}\Phi^{*2} \right), \\
i\hbar\dot{\tilde{m}} &= g(2\tilde{n} + 1/V)\Phi^2 + 4\left(-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}} - \mu + 2gn + \frac{g}{4}(2\tilde{n} + 1/V) \right)\tilde{m},
\end{aligned}
\qquad (2.2)
$$

where we have introduced the volume V of the gas in order to ensure the correct dimensions. In Eqs.(2.2), Φ is the order parameter, n_c the condensate density ($n_c = |\Phi|^2$), $\tilde{n}$ the non-condensed density (or thermal cloud) and $\tilde{m}$ is the anomalous density. The quantity $n \equiv n_c + \tilde{n}$ is the total density.

The TDHFB equations with a general Hamiltonian H were derived in [16]. The properties discussed here and in [12] were established there in their general forms. These equations were obtained using the Balian-Vénéroni variational principle[13], with a gaussian trial density operator (that is, an exponential operator of a quadratic form) in the creation and annihilation operators. The result was a set of coupled evolution equations for the expectation values $\langle a \rangle$, $\langle a^+ a \rangle - \langle a^+ \rangle \langle a \rangle$ and $\langle aa \rangle - |\langle a \rangle|^2$. When one identifies these quantities respectively with the order parameter Φ, the non-condensed density $\tilde{n}$ and the anomalous density $\tilde{m}$, and when one restricts H to the class (2.1), the equations (2.2) follow.

The TDHFB equations couple in a consistent and closed way the three densities. They should in principle yield the general time, space and temperature dependence of the various densities. Furthermore, they obviously constitute a natural extension of the Gross-Pitaevskii equation[14]. They are not only energy and number conserving, but also satisfy the Hugenholtz-Pines theorem (see below) which leads to a gapless excitation spectrum in the uniform limit. Moreover, the two last equations in (2.2) are not totally independent since $\tilde{n}$ and $\tilde{m}$ are related by the "unitarity" relation[12]:

$$I = (1 + 2V\tilde{n})^2 - (2V|\tilde{m}|)^2 , \qquad (2.3)$$

where the Heisenberg parameter I (which is always ≥ 1) is a measure of the temperature, the lower limit being the zero temperature case. For instance, for a thermal distribution at equilibrium, I writes as $I = \coth^2 (\hbar\omega_0/2k_B T)$, where ω_0 is the average frequency of the trapping field[12] [1] . We therefore see that upon replacing $\tilde{n}$ by its expression given in (2.3), the temperature appears explicitly in the equations.

It is to be mentioned that the TDHFB equations have also been derived by several authors using different variational formulations[17, 18]. In the first reference, the authors have obtained a set of equations very similar to ours. In fact, we can show that our equations can be deduced from theirs by taking the diagonal elements ($\mathbf{r} = \mathbf{r}'$) of the equations (B1), (B2) and (B3) [2] of ref.[17].

The static solutions, which are the object of our study in this work, are obtained by setting to zero the right hand sides of (2.2). At zero temperature, the standard TF

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[1]In fact, one can show that for a system of energy E, $\sqrt{I} = 1 + 2 f_B(E)$, where f_B is the Bose-Einstein distribution.

[2]There is however a factor 1/2 missing from (B3).

limit[19] amounts to neglecting the kinetic (or Δ) term in the Gross-Pitaevskii equation. This is particularly satisfied for strong interacting regimes or large atom numbers. At finite temperature and below the transition, since there are two phases (condensed and non condensed) which coexist, one has to provide a complementary recipe for what we shall call the finite temperature TF limit. First, neglecting the kinetic energy of the condensate remains a justifiable approximation since the atoms are slowed down in order to obtain condensation. On the other hand, $\tilde{m}$ is believed to be an extremely small and slowly varying function whatever the temperature is (recall that it describes the correlations between the condensed and non-condensed phases). Hence, one may in a first approximation safely neglect $\Delta\tilde{m}$. Heuristically, one may argue that, since the equations for n_c and $\tilde{m}$ contain almost comparable operators, h_0 and $h_0 + g(n_c + (1 + 2V\tilde{n})/4V)$, where h_0 is the self-consistent mean field hamiltonian $h_0 = V_{\text{ext}}(r) - \mu + gn_c + 2g\tilde{n}$, the TF condition $h_0 >> T$ (T being the kinetic operator), if fullfilled for n_c shouldf also be satisfied for $\tilde{m}$. For this approximation to be consistent, n_c and $\tilde{m}$ should vary on the same characteristic length, which is indeed the case as we will show later.

Before proceeding further, it is important to notice at this point that a kinetic-like term of the thermal cloud does not appear explicitly in the equations but is rather hidden in the third equation of (2.2). Indeed, the kinetic term of the thermal cloud is related to the second derivative of the anomalous density. Differentiating (2.3) yields a relation of the form:

$$\Delta\tilde{n} \sim (\nabla|\tilde{m}|)^2 - (\nabla|\tilde{n}|)^2 + |\tilde{m}|\Delta|\tilde{m}|, \tag{2.4}$$

which shows in particular that neglecting $\Delta\tilde{m}$ does not necessarily mean neglecting $\Delta\tilde{n}$. That is precisely the recipe that we shall adopt below.

With this finite temperature prescription, the static equations corresponding to (2.2) now write

$$
\begin{aligned}
&\left(V_{\text{ext}}(r) - \mu + gn_c + 2g\tilde{n}\right)\Phi + g\tilde{m}\Phi^* = 0, \\
&\tilde{m}^*\Phi^2 - \tilde{m}\Phi^{*2} = 0, \\
&\left(V_{\text{ext}}(r) - \mu + 2gn + \frac{g}{4V}(2V\tilde{n} + 1)\right)\tilde{m} + \frac{g}{4V}(2V\tilde{n} + 1)\Phi^2 = 0,
\end{aligned}
\tag{2.5}
$$

These equations are naturally gapless and satisfy the Hugenholtz-Pines theorem[9]. Indeed, owing to the second equation in (2.5), one can easily show that at zero momentum, the relation $\mu = g(n + \tilde{n} - |\tilde{m}|)$ is clearly satisfied without adding further assumptions, as is usually performed[9].

In order to solve these equations, we may distinguish two rather different situations. The first one is for $T = 0$. When all the atoms are condensed, $\tilde{n} = \tilde{m} = 0$, and n_c equals the total density n of the gas. Omitting the trivial solution with $n_c = 0$, one may take into account just the first equation in (2.5), since we consider a gas without a quantum cloud.

Indeed, within the present set of equations, it is an approximation (although justifiable) to ignore the quantum depletion at $T = 0$. The last two equations in (2.5) become therefore meaningless, and we are left with a simple expression for the condensate density

$$n_c(r) = -\xi(r) = \frac{1}{g} \left(\mu - V_{\text{ext}}(r) \right). \tag{2.6}$$

Upon defining the oscillator length $a_0 = (\hbar/m\omega_0)^{1/2}$ and the s-wave scattering length $a = mg/4\pi\hbar^2$, we obtain for a spherical trapping potential $V_{\text{ext}}(r) = \frac{1}{2}m\omega_0^2 r^2$, the condensate radius R and the reduced chemical potential $\nu_0 = \mu/\frac{1}{2}\hbar\omega_0$ for a gas of N bosons as

$$\frac{R}{a_0} = \left(15N\frac{a}{a_0} \right)^{1/5}, \tag{2.7}$$

$$\nu_0 = \left(15N\frac{a}{a_0} \right)^{2/5}. \tag{2.8}$$

The preceding expressions show that the spreading of the condensate depends essentially on the balance between the self-interactions and the trapping potential. These results have also been obtained by many other authors, see e.g. [8, 11, 12].

When $0 \leq T < T_{\text{BEC}}$, we have of course $n_c \neq 0$ and $\tilde{n} \neq 0$. Let us introduce the parametrization $2V\tilde{n} + 1 = \sqrt{I}\cosh\sigma$, $2V|\tilde{m}| = \sqrt{I}\sinh\sigma$, which automatically endows the relation (2.3). Then, from the third equation in (2.5), one obtains a simple equation for $X = e^\sigma$:

$$3X^4 - 4X^2 + 1 + \frac{4Vn_c}{\sqrt{I}}\left(X^2 - 3 \right)X = 0, \tag{2.9}$$

from which one extracts $\tilde{n}$ and $|\tilde{m}|$ as functions of n_c. Next, one uses these expressions in the first equation (2.5) to get the condensate density

$$n_c(r) = -\xi(r) - \frac{1}{V}\left(\frac{X + 3X^{-1}}{4}\sqrt{I} - 1 \right). \tag{2.10}$$

What is remarkable is that the sole acceptable solution of equation (2.9) is a bounded function of $\eta = Vn_c/\sqrt{I}$. It is represented on figure 1.

Due to this behavior, one can easily show that the quantity $\frac{X+3X^{-1}}{4}$ which appears in (2.10) is almost independent of n_c and becomes rapidly close to unity. Indeed, since equation (2.10) may also be rewritten as $\eta = \frac{(1-V\xi)}{\sqrt{I}} - (X + 3X^{-1})/4$, its solution provides the typical linear behavior shown in figure 2.

Hence, one may safely approximate (2.10) by

$$n_c(r) \simeq -\xi(r) - \frac{1}{V}\left(\sqrt{I} - 1 \right). \tag{2.11}$$

In fact, one can check that the relative error between the two expressions (2.10) and (2.11) is less than 1%. Finally, since $\sqrt{I}$ does not depend on space, the result (2.11)
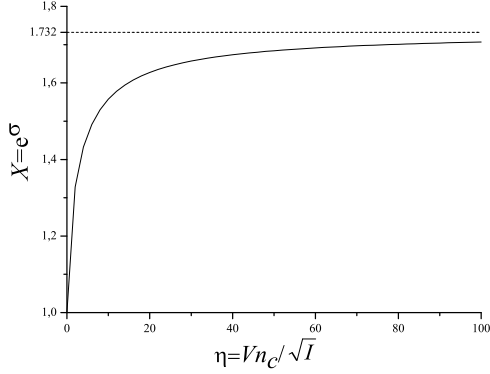
Fig.1: Solution of Eq.(2.9) vs. the dimensionless condensate density.
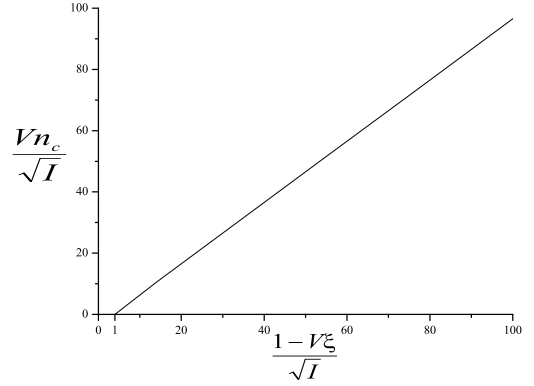

Fig.2: Plot of the solution of eq.(2.10) showing a typical linear behavior.

shows that the finite temperature correction to the Thomas-Fermi profile (2.6) is simply a space-independent (but temperature dependent) shift. This shift may be absorbed in a redefinition of the chemical potential which now writes

$$\mu = V_{\text{ext}}(R) + \frac{g}{V}\left(\sqrt{I} - 1\right), \tag{2.12}$$

where R is the condensate radius. The condensate density finally writes in the suggestive form

$$n_c(r) = \frac{V_{\text{ext}}(R) - V_{\text{ext}}(r)}{g}, \tag{2.13}$$

which is formally the zero temperature TF profile. It is then easy to show that the condensate radius takes also a simple form

$$\frac{R}{a_0} = \left(15 N_c \frac{a}{a_0}\right)^{1/5}, \tag{2.14}$$

but now, it is the number of condensed atoms N_c which is involved and not the total number of atoms. The same conclusion may be drawn for the chemical potential (2.12). Hence, our finite temperature prescription for the TF approximation provides natural extensions of the zero temperature expressions, since the Thomas-Fermi parameter is now $N_c a/a_0$ instead of Na/a_0.

In order to apprehend better these results, let us compute the remaining unkown quantities, such as the non condensed and the anomalous densities. To this end, and in order to obtain tractable expressions, we find it more convenient to use the simple fit

$$X = \frac{\sqrt{3}\eta + 2/3}{\eta + 2/3}, \tag{2.15}$$

(instead of the full analytical solution of equation (2.9)) which reproduces correctly the solution X plotted in figure 1 with a residual error less than 0.1%. Upon rewriting

equation (2.13) in the form $\eta = \eta_0(1 - x^2)$, with an obvious definition of η_0, we obtain the non condensate density

$$\tilde{n}(x) = \frac{1}{2V}\left\{\frac{\sqrt{I}}{2}\left(\frac{\sqrt{3}\eta_0(1-x^2)+2/3}{\eta_0(1-x^2)+2/3} + \frac{\eta_0(1-x^2)+2/3}{\sqrt{3}\eta_0(1-x^2)+2/3}\right) - 1\right\}, \qquad (2.16)$$

and the anomalous density

$$|\tilde{m}|(x) = \frac{1}{2V}\frac{\sqrt{I}}{2}\left(\frac{\sqrt{3}\eta_0(1-x^2)+2/3}{\eta_0(1-x^2)+2/3} - \frac{\eta_0(1-x^2)+2/3}{\sqrt{3}\eta_0(1-x^2)+2/3}\right), \qquad (2.17)$$

as functions of the reduced radial distance $x = r/R$. In figures 3 and 4, we show typical density profiles (in reduced units) for $\eta_0 = 1$.
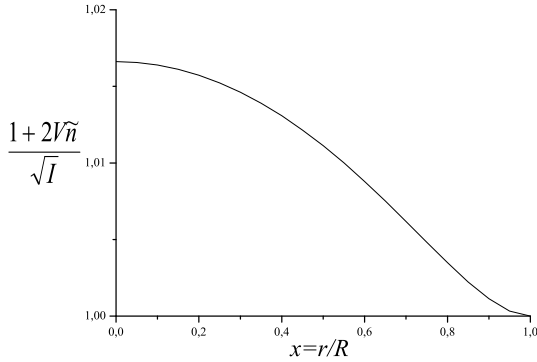
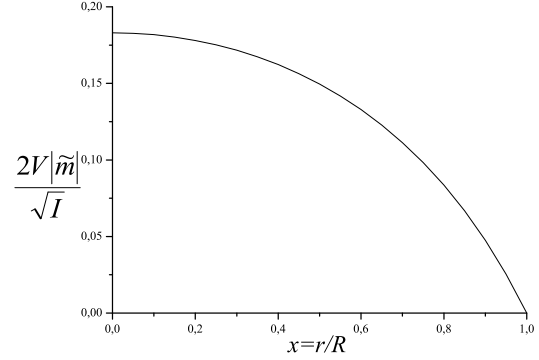**Fig.3:** Noncondensate density vs. the radial distance.   **Fig.4:** Anomalous density vs. the radial distance.

It is interesting to notice that, within our TF approximation, the figure 3 is qualitatively consistent with the profile of the thermal cloud as depicted by Gerbier *et al*[15]. It also predicts that the thermal cloud does not vanish at the boundaries of the condensate which is also compatible with the experimental results since it is widely known that condensed atoms are surrounded by the thermal cloud. What is less known (even experimentally) is the anomalous density (figure 4). This quantity behaves quite differently from the thermal cloud and is clearly dominated by a TF-like shape. In contrast with the thermal cloud, the anomalous density vanishes at the boundaries which is also plausible since the condensate vanishes there. Furthermore, we observe that n_c, $|\tilde{m}|$ and $\tilde{n}$ vary on the same length scale (R) which justifies *a posteriori* our previous assumption.

In order to obtain more quantitative results, one must determine N_c by using the normalization condition. We get easily the relation

$$1 + 2N = 2N_c + \sqrt{I}g(s), \qquad (2.18)$$

where

$$g(s) = \frac{2}{\sqrt{3}} + (\sqrt{3}-1)s\left\{1 - \frac{3}{2}\sqrt{s+1}\,\text{arc}\tanh\frac{1}{\sqrt{s+1}} + \frac{1}{2}\sqrt{\frac{s}{\sqrt{3}}+1}\,\text{arc}\tanh\frac{1}{\sqrt{\frac{s}{\sqrt{3}}+1}}\right\}, \qquad (2.19)$$

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with $s = 4\sqrt{I}/15N_c$. But since the function $g(s)$ satisfies $1 \leq g(s) \leq 2/\sqrt{3}$, the equation (2.18) is approximately solved to yield, to a very good accuracy, the simple result

$$N_c \simeq N - \frac{\sqrt{I} - 1}{2}. \tag{2.20}$$

All the unknown quantities may now be determined in terms of N and $\sqrt{I}$ alone. The corresponding results will be discussed in the next section.

3   Results and Discussions

First of all, the condensate radius (2.14) may be written as

$$R = R_{\mathrm{TF}} \left(\frac{N_c}{N} \right)^{1/5}, \tag{3.1}$$

where R_{TF} is the zero temperature result given by equation (2.7). Figure 5 represents the condensate radius (in units of R_{TF}) as a function of the condensate fraction and we notice in particular the compression of the condensate when reducing N_c/N (that is increasing the temperature). This effect is by now a well established experimental result [15] and is attributed to the thermal cloud. The same effect of compression is observed on figure 6 for the central condensate density $n_c(r = 0)$ but it is more pronounced due to the power law of 2/5 (see 2.13) instead of 1/5 for the condensate radius. To be more precise, let us choose generic values for the number of atoms and the interaction strength ($N = 10^5$ and $a/a_0 = 0.5 \, 10^{-3}$) and plot the various densities (in units of the oscillator volume a_0^3) versus the radial distance (in units of $R_{\mathrm{TF}} = 3.758a_0$) for a condensate fraction ranging from 5% up to 60%.
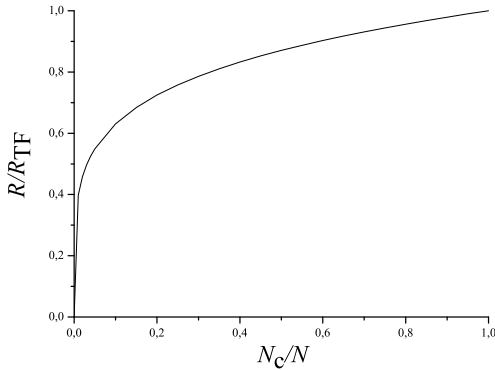
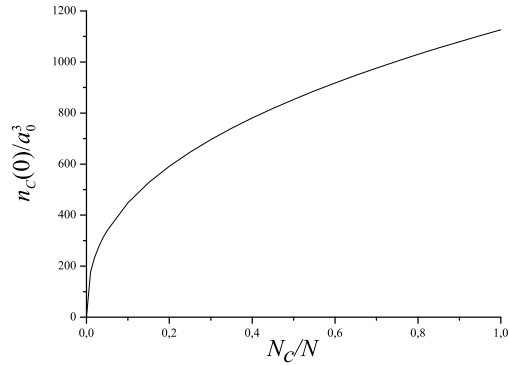**Fig. 5**: Condensate radius vs. the condensate fraction.

Fig. 6: Central density vs. the condensate fraction.

The figure 7 shows typical Thomas-Fermi profiles for the condensate density, even for low condensate fraction. This is of course what one may expect on general grounds

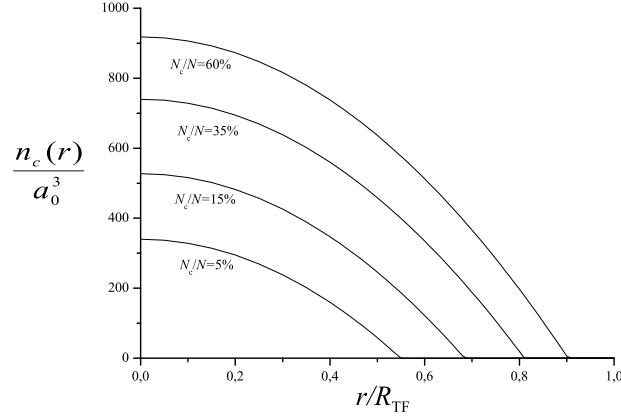in the TF regime. Moreover, the effect of compression of the condensate is also clearly visible here.

Fig. 7: Condensate density vs. the radial distance for varying condensate fraction for $N=10^5$ and $a/a_0=0.5 \ 10^{-3}$.

The noncondensate density (from which we have substracted a constant $\tilde{n}(R)$ for clarity) is plotted on figure 8 with the same units as before. The information which is
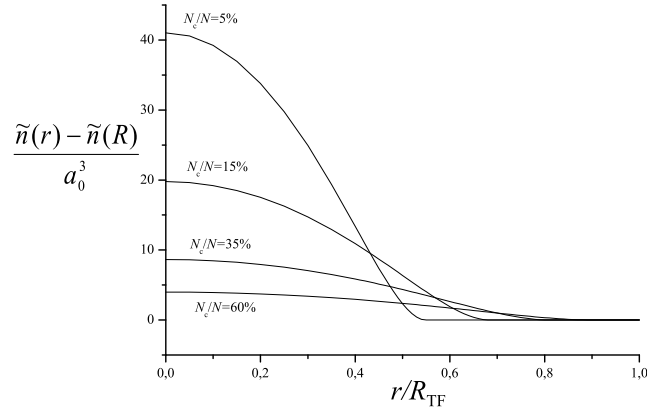

Fig. 8: Noncondensate density vs. the radial distance for varying condensate fraction for $N=10^5$ and $a/a_0=0.5 \ 10^{-3}$.

added here with respect to figure 3 is the temperature dependence which appears via the condensate fraction. As noted earlier, the experimental result[15] is well reproduced qualitatively for the whole range of condensate fraction[3]. In particular, we notice that when increasing the condensate fraction, the thermal cloud tends to spread and flatten.

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[3] Although, in order to compare exactly with the experimental results, one must include an overall scale factor due to the finite ballistic expansion time.

On the other hand, the thermal cloud takes on a (small but) finite value for $r \geq R$. Even if this behavior is less intuitive, it is not very surprising since we do know that neglecting the second order derivatives amounts to making a cut of the densities at the boundaries. It is indeed a limitation of the TF approximation at the boundaries[20]. The tail should be reproduced when one reinjects the second derivatives in the equations.
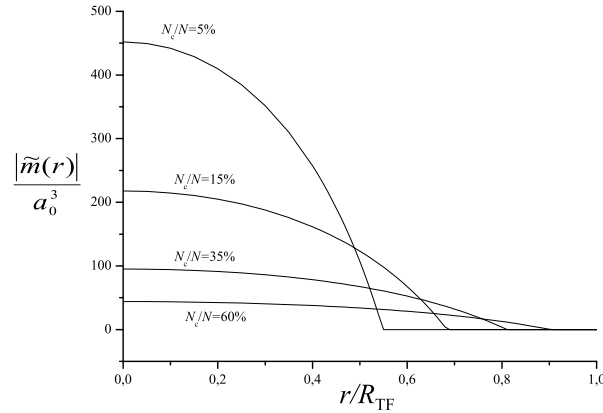

Fig. 9: Anomalous density vs.the radial distance for varying condensate fraction for $N=10^5$ and $a/a_0=0.5 \; 10^{-3}$.

Finally, we plot on figure 9 the anomalous density. To our knoweledge, this quantity was never measured experimentally, and it is interesting that our calculations predict a very simple and yet intuitive behavior as well which remains of course to be confirmed.

4 Concluding Remarks

We present in this paper a finite temperature analysis of the static TDHFB equations (derived in a previous paper) in the Thomas-Fermi limit for a gas of bosons in a harmonic trap.

At zero temperature, we obtain familiar expressions for the chemical potential and the condensate radius. The standard Thomas-Fermi profile for the condensate density is also recovered.

At finite temperatures and below the transition, since there are two phases, one should provide a prescription for the TF limit. We propose such a recipe (maybe the simplest) which consists in neglecting the second order derivatives of the condensate density and the anomalous density. The underlying idea is that, although the anomalous density is necessary for the coherence of the equations, it is believed to be a very small

and hopefully a very smooth quantity. We therefore obtain analytical expressions for the condensate density, the condensate radius, the chemical potential and the condensate fraction as functions of the temperature. Our expressions appear as natural extensions of the zero temperature TF limit, since the relevant parameter which controls the approximation becomes $N_c a/a_0$ instead of Na/a_0.

Most importantly, we derive quite simple expressions for the noncondensate density and for the anomalous density, which we plot as functions of the condensate fraction and draw many conclusions. First of all, the condensate profile is almost of the TF shape of which the spatial extension and the heights are controlled by N_c/N. Furthermore, the compression of the condensate by the thermal cloud with increasing temperature is clearly visible. On the other hand, the noncondensate density profile is qualitatively consistent with the condensate fraction dependence observed in recent experiments. In particular, the thermal cloud tends to spread and flatten with increasing temperature. The calculated anomalous density, although not yet observed experimentally, shows also a very intuitive behavior; it is maximal at the center of the trap and zero at the boundaries. The tendency to spreading and flattening with increasing temperature is also observed here.

At the borders of the trap (where the condensate density vanishes) and for a given temperature, the non condensate density takes on a finite value which is a quite abrupt behavior. Athough this meets the fact that the thermal cloud is actually surrounding the condensate, it is to by no means conclusive. But this is also a shortocoming of the TF approximation as a whole since it is known to break down at the boundaries of the condensate. Indeed, reinjecting the second derivatives of the densities will certainly entail a more physical behavior.

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